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Investigating the effect of solvent on anti-antioxidant properties of *Sesamum indicum* seeds

Mercy Badu * , Gilsonda Akweley Kordei Attuquaye , Azanlerigo Emmanuel

Department of Chemistry, Kwame Nkrumah University of Science and Technology, Kumasi, Ashanti Region, UPO PMB, Ghana

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ABSTRACT

Dietary phytochemicals are important bioactive compounds that can scavenge reactive oxygen species. These essential compounds may have antioxidant properties which are known to play a significant role in the treatment and prevention of many chronic diseases. Sesame, an oil-bearing seed, is a well-known promising source of food with both nutritional and therapeutic benefits. As a result, the study aimed to evaluate the antioxidant properties of different solvent extracts of Sesame seeds and to analyse the bioactive compounds present. The seeds were obtained from the local farmers and prepared for analysis. The bioactive compounds present in the seeds were extracted using hexane, ethyl acetate, ethanol, and water. The total phenolic content (TPC), the condensed tannin content (CTC), the total antioxidant capacity (TAC), and the 2,2-Diphenyl-1 picrylhydrazyl (DPPH) radical scavenging assay were also determined using standard methods. Two chemometric methods, hierarchical cluster analysis (HCA) and Pearson correlation, were employed to evaluate the interdependence of the various parameters and the antioxidant activity. Anti-nutrients such as saponins, alkaloids, phytates, and oxalates were also analysed from the powdered seeds. The study results revealed the presence of anti-nutrients such as phytate (7.691 \pm 0.8576 mg/g), oxalate (1.501 \pm 0.1375 mg/g), saponins (21.33 \pm 4.619 mg/g) and alkaloids $(317.33 \pm 30.29 \text{ mg/g})$. The study also revealed that the aqueous extract exhibited the highest TPC (17.12 \pm 0.041 mg GAE/g of dried extract, p < 0.05) and CTC (64.27 \pm 4.711 mg CE/g of dried extract, $p < 0.05$). Ethanol and hexane had a similar total phenolic content (14.83 \pm 0.123 and 14.66 ± 1.474 mg GAE/g of dried extract, respectively, p *<* 0.05Ethyl acetate had the lowest TPC content. Ethanol extracts had the highest antioxidant activity with a TAC value of 232.6 \pm 6.267 mg/g AAE and a DPPH scavenging activity of IC₅₀ of 52.81 \pm 2.30 μ g/mL. A good correlation (p *<* 0.05) was established between the extracts' TPC, CTC, TAC, and DPPH radical scavenging activity. Chemometric analysis from the study showed no significant connection between the radical scavenging activity of TPC and DPPH. From the results obtained, it can be concluded that the bioactive compounds present in the sesame seed and their subsequent antioxidant properties are dependent on the nature of the solvent used for extraction.

1. Introduction

Dietary phytochemicals are important bioactive compounds, that have the ability to scavenge reactive oxygen species. These essential compounds possess antioxidant properties which are known to play a significant role in the treatment and prevention of many

Corresponding author.

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E-mail addresses: mbadu0@gmail.com (M. Badu), gattuquaye@gmail.com (G.A.K. Attuquaye), azanlerigoemmanuel@gmail.com (A. Emmanuel).

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chronic diseases. Phenolic compounds have been reported widely in the literature to have health benefits such as anticancer, antiaging, and antioxidant properties [[1](#page-7-0)]. Plant polyphenols are being studied extensively as important naturally occurring antioxidant compounds [[2](#page-7-0)]. Polyphenolic compounds exhibit antioxidant activity as a result of their redox properties which allows them to act as reducing agents, hydrogen donors, singlet oxygen quenchers, and metal chelators [[3](#page-7-0)]. This unique property enables them to protect tissues from radical oxidative damage. Most edible plants show high medicinal value based on the composition of their phytochemical constituents. Some essential phytochemical compounds reported include phenolics, tannins, flavonoids, alkaloids, and glycosides [\[4\]](#page-7-0). Daily intake of foods containing significant antioxidant compounds has been associated with preventing various diseases related to oxidative/nitrosative stress, including cardiovascular diseases, neurological disorders, and cancer [\[5](#page-7-0)–7]. Numerous epidemiological studies have revealed the impact of consuming plant phenolics and their benefit to good health and well-being [8–[10](#page-7-0)].

Sesame (*Sesamum indicum* L.) is a well-known oilseed worldwide. Sesame belongs to the genus *Sesamum* and the family *Pedaliaceae*. The plant thrives in semi-arid conditions such as in Asia and Africa. In Ghana, the sesame plant is largely cultivated in the Northern Savanna areas for the leaves and oils from the seeds. However, reports show that sesame seeds have several important uses and not only for the production of edible oil $[7,11,12]$ $[7,11,12]$. Sesame seeds have been used as an important ingredient in traditional Chinese medicine, nutraceuticals and other pharmaceutical products. The seeds contain essential bioactive compounds such as phenolics, tocopherols, vitamins, phytosterols, and fatty acids, which are essential to the human body. In addition to the numerous benefits of sesame seed oil, the seed meal obtained after extraction of the oils can be used as a source of protein to support the nutritional value of infants as well as animal feed products. Again, the sesame seed meal has been reported to contain a variety of important phytochemicals. As a result of the presence of these bioactive compounds, sesame seeds can be adopted for pharmaceutical use. The sesame seeds have shown properties of anticancer activities, lowering of cholesterol levels in the blood, and antioxidant activities and their therapeutic benefits have been widely studied [[3](#page-7-0),[13\]](#page-7-0).

Like all other oilseeds, sesame seeds also contain other phyto-constituents that have anti-nutritional properties and hence inhibit the body's ability to absorb essential nutrients. Such compounds include phytates, oxalates, cyanates, alkaloids, saponins, tannins, etc. To achieve optimum access to the essential compounds found in the sesame seeds, there is a need to consider the type of solvent used for the extraction of the compounds. For effective recovery of phenolic compounds, polar solvents such as water, methanol, and ethanol have been used [[14\]](#page-7-0). Additionally, lipids and lipid-soluble compounds have been reported to play a significant role in protecting cells from oxidative damage, this contributes to the body's overall antioxidant defense system [[15\]](#page-7-0). The current study aims to investigate the antioxidant properties of different solvent extracts of sesame and to analyse the bioactive compounds present. Solvents with different polarities were employed. These include; water, ethanol, ethyl acetate and n-hexane. The purpose of using the different solvents was to investigate the effect of the polarity of the solvent on the yield of phenolic compounds extracted and also to determine the dependence of antioxidant capacity on the phenolic compounds found in the sesame seeds. Chemometric techniques, including unsupervised hierarchical cluster analysis (HCA) and Pearson bivariate analysis, were applied to evaluate and develop a classification model to determine the correlations between the bioactive compounds and antioxidant activities.

Whilst many studies usually focus on using a single solvent extraction method, however, our research evaluates the antioxidant properties and bioactive compounds of sesame seeds using different kinds of solvents (hexane, ethyl acetate, ethanol, and water). That is conducting a comprehensive comparison provides a deeper understanding of how different solvents may have significant effect on the extraction efficiency of phenolic compounds and antioxidant activity. Additionally, the use of hierarchical cluster analysis (HCA) and Pearson correlation to evaluate the interdependence of various parameters and antioxidant activity adds a statistical and analytical depth to the study. This approach helps in identifying significant correlations and patterns that might not be evident through simple descriptive statistics.

2. Materials and methods

2.1. Sample collection and preparation

The study sample was collected from farmers in the Upper East Region of Ghana during the harvest season from November 2020 to June 2021. They were identified and authenticated by a botanist in the Department of Herbal Medicine, Faculty of Pharmacy and Pharmaceutical Sciences, Kwame Nkrumah University of Science and Technology (KNUST). The seeds were then cleared of all extraneous matter by sorting and sieving, and they were air-dried, milled, and kept in an air-tight container until ready for use.

2.2. Reagents and chemicals

2,2-Diphenyl-1-picrylhydrazyl (DPPH), catechin, gallic acid, ascorbic acid, vanillin, and Folin-Ciocalteau (FC) reagents and all other chemicals and reagents were purchased from Sigma-Aldrich, UK.

2.3. Extraction

The powdered plant materials (300 g) each were cold macerated in 700 ml of the respective solvent (water (aqueous), ethanol, ethyl acetate, and hexane) for 72 h. The extracts were then filtered using a CHMLAB Group medium-fast F1001 grade filter paper. The filtrate was lyophilized using a freeze dryer (Power dry LL3000, Thermo Electron Corporation, Czech Republic). The percentage yield was calculated as expressed in equation [\(1\).](#page-2-0) The dried extract was kept in a desiccator for subsequent use. The extracts were coded using the name of the seed and that of the solvent; SA (Sesame aqueous), SE (Sesame ethanolic), SETAC (sesame ethyl acetate), and SH (sesame hexane)

Percentage yield of dried extract =
$$
\left(\frac{\text{weight of dried extract}(g)}{\text{weight of sample used}(g)}\right)X\,100
$$
 (1)

2.4. Phytochemical analysis (anti-nutrients)

2.4.1. Saponins

The amount of saponins was determined using the method described by (16) with some modifications. 1.25 g of the powdered plant sample was added to 25 mL of 20 % ethanol and heated with continuous stirring in a water bath at 55 ℃ for 4 h. It was filtered, and the residue was extracted with another 25 mL of 20 % ethanol. The filtrates were combined and reduced to 40 ml in a water bath at 90 ◦C. The concentrate was introduced into a separate funnel and vigorously stirred with 20 mL of diethyl ether. The ether layer was discarded, and the aqueous layer was retained. 60 mL of n-butanol was added to the retained aqueous layer in the separation funnel and vigorously stirred. The butanol layer was retained and shaken twice with 10 ml of 5 % aq. NaCl. The remaining solution was collected, evaporated in a water bath, and dried to a constant weight in an oven at 40 ℃. The saponin content was calculated using the following equation.

Saponin content =
$$
\left(\frac{\text{weight of residue } (mg)}{\text{weight of the original sample } (g)}\right)
$$
 (2)

2.4.2. Alkaloids

The powdered plant material (1.25 g) was mixed with 50 ml of 10 % acetic acid in ethanol, covered, and left to stand for 4 h. It was filtered, and the filtrate was concentrated in a water bath of about 15 mL. Concentrated ammonium hydroxide was added in drops until precipitation was complete. The solution was left to settle, washed with dilute ammonium hydroxide, and filtered. The residue was collected and dried to a constant weight $[16]$ $[16]$. The alkaloid content was calculated using;

Alkaloid content =
$$
\left(\frac{\text{weight of residue (mg)}}{\text{weight of the original sample (g)}}\right)
$$
 (3)

2.4.3. Oxalates

Oxalates in the powdered plant sample were quantified using a method described by (16). Exactly 1 g of the powdered plant sample was weighed in a beaker, and sulfuric acid (75 mL; 1.5 N) was added. The mixture was stirred continuously for 1 h using a magnetic stirrer and filtered. The filtrate (25 mL) was titrated hot against 0.1 M KMnO₄ until a pink colour formed that persisted for about 30 s at the endpoint.

The oxidative content of the sample was calculated as = (titre value × 0.9004) mg/g\n
$$
(4)
$$

2.4.4. Phytates

The phytate content of the powdered plant sample was evaluated using a method described by [[16](#page-7-0)] with some modifications. 2 g of the sample was weighed in a conical flask and HCl (50 mL; 2% v/v) was added. The mixture was stirred continuously for 3 h and filtered. The filtrate (25 mL) was measured into a conical flask, 50 mL of distilled water was added to the filtrate, and 5 mL of 0.3 % ammonium thiocyanate indicator was added. The solution mixture was titrated against 0.00195 g/ml iron(III) chloride solution until a brownish-yellow colour was observed that persisted for approximately 5 min. The phytate content was calculated using the following equation;

$$
Phytate content (mg / g) = \frac{8.24 (titre value)}{weight of sample taken}
$$
\n(5)

2.5. Antioxidant activity assays

2.5.1. Total phenolic content (Folin-Ciocalteau assay)

The reference compound gallic acid solutions (1.5625–200 μg/mL) were prepared, and 0.5 mL were measured in test tubes and mixed with 2.5 ml of Folin-Ciocalteau (FC) reagent (10 %) and neutralised with 2 ml of aqueous Na₂CO₃ (75 mg/mL). The extracts (0.5 mL) were taken through the same procedure as the reference compound. The reaction mixtures were incubated at 50 ◦C for 10 min, and the absorbances were measured at 760 nm on the multimode microplate reader. The total phenolic content determined from the equation of the line of the calibration curve was expressed as equivalent gallic acid (mg GAE/g of extract) [[8](#page-7-0)].

2.5.2. Condensed tannins content

The condensed tannin content was colorimetrically evaluated using the vanillin-HCl assay reported by [[17\]](#page-7-0) with some modifications. Extracts (0.5 mL) were placed in test tubes wrapped in aluminium foil due to the light-sensitive nature of the experiment. Freshly prepared vanillin methanol reagent (3 mL; 4 %, w/v) and 1.5 mL of concentrated HCl were added to the extracts and thoroughly mixed. The reaction mixtures were kept in the dark at room temperature for 15 min, and absorbance were read at 500 nm.

Table 1

Results for the percentage yield of the different crude extract.

Catechin solutions (1.5625–200 μg/mL) were prepared and taken through the same procedure, and absorbances were measured at the same wavelength. The condensed tannin content of the plant extracts was determined from the calibration curve and expressed as mg/g CE (Catechin Equivalents).

2.5.3. Total antioxidant capacity (Phosphomolybdate assay)

Ammonium molybdate (4 mM), disodium hydrogen phosphate (28 mM), and sulfuric acid (6 mM) were used in the preparation of the reagent solution. The extract solutions (500 μg/mL: 1 mL) were taken into labelled test tubes, and 3 mL of the reagent solution was added to each. Ascorbic acid solutions (1.5625–200 μg/mL) were prepared, and 3 mL of the reagent solution was added to 1 mL of the solutions. The reaction mixtures were incubated at 95 \degree C for 90 min and absorbance were measured at 695 nm using the Synergy H¹ Hybrid Multi-Mode Microplate Reader, BioTek Instruments to plot the calibration curve. The total antioxidant capacity of the extracts determined from the linear equation of the calibration curve was expressed as mg of ascorbic acid equivalent (AAE) per g of the extract [\[18](#page-7-0)].

2.5.4. DPPH free radical scavenging assay

The ability of the extracts to scavenge free radicals and ascorbic acid (reference compound) was evaluated using a method reported by [[19\]](#page-7-0). Extract solutions (31.25–1000 μg/mL, 1 mL) were added to 3 mL of DPPH (20 mg/L) in labelled test tubes. The reaction mixtures were incubated in the dark at room temperature for 30 min. The reaction process was repeated for the reference compound, ascorbic acid, of different concentrations (1.5625–200 μg/mL). The absorbance of the residual DPPH was determined at 517 nm in the multimode microplate reader. The DPPH free radical scavenging activity was calculated from the following equation:

% DPPH radical scavenging activity =
$$
\left(1 - \left(\frac{Abs\ of\ sample}{Abs\ of\ control}\right)\right)
$$
 x 100% (6)

The percentage of DPPH radical scavenging activity was plotted against the log concentration of the reference compound and extracts. The concentration required to eliminate 50 % of DPPH radicals was expressed in IC_{50} .

2.6. Statistical evaluations

The results are shown as means \pm standard deviation (SD) values. The statistical analysis was done by One-way ANOVA using Minitab®19.2020.1 (copyright© 2012 Minitab Inc., Philadelphia, PA, USA) and GraphPad Prism version 6. The differences between treatments and the standard data were considered significant at p *<* 0.05 using Tukey's HSD test. A chemometric approach, the unsupervised hierarchical cluster analysis (HCA), was performed using Minitab®19.2020.1 (copyright© 2012 Minitab Inc., Philadelphia, PA, USA). The HCA method was utilised to assess the relationships between the *S. indicum* extracts. The squared Euclidean distance and Ward's linkage method were used to generate the dendrogram for the plant extract samples determined for each cluster. Pearson correlation was also undertaken using Minitab®19.2020.1 (copyright© 2012 Minitab Inc., Philadelphia, PA, USA) to evaluate the possible relation between TPC, CTC, TAC, and antioxidant activity of the studied extracts.

3. Results and discussion

3.1. Percentage yield of extracts

The selection of solvents is crucial in the extraction process, the nature of the solvent, and the quantity and quality of extracts and compounds extracted. In the current study, the samples were directly extracted with the selected solvents to ascertain the overall effect of the solvent on the various phytochemicals found. To achieve the full benefit of sesame seeds, the bioactive compounds present must be extracted using an appropriate solvent system. In the current study, the dried seed samples were extracted using water and ethanol (polar); ethyl acetate (mid-polar) and hexane (non-polar). The yield of extracts obtained was estimated using Equation [\(1\),](#page-2-0) and the results were expressed as a percentage dry weight of extract/weight of sample used. The yield ranged from 11.90 to 49.34 % as presented in Table 1.

The results showed a significant difference (p *<* 0.05) in the percentage yield of the extracts obtained, showing the effect of the nature of solvent on the extraction process. Among the solvents used, hexane gave the highest yield (49.34 %) followed by ethyl acetate, and water gave the lowest yield (11.90 %). The hexane solvent was used to extract the oil content of the sesame seeds which also represent mostly the non-polar compounds present in the seeds. Hexane, has been used as accepted as on the solvents for large scale oils extraction [\[20](#page-7-0)]. Whilst water and ethanol were expected to extract the polar components, mostly the polyphenols.

All data were recorded as mean and standard deviation. Means in the same column that do not share the same letter are significantly different p *<* 0.05.

Table 3

Shows the results for total phenol content (TPC), condensed tannin content (CTC), total antioxidant capacity (TAC), and DPPH Free Radical Scavenging Activity of the seed extracts.

Values are represented as mean \pm standard deviation (n = 3); Statistical significance: The means in columns that do not share the same superscript letter are significantly different. ($p < 0.05$). (mg GAE)/g = milligram of gallic acid equivalent per gram of dried extract; mg CE)/g = milligram of catechin equivalent per gram of dried extract; $(mg AAE)/g =$ milligram of ascorbic acid equivalent per gram of dried extract; ND = not detected.

Polyphenolic compounds are characterized by an aromatic ring and a hydroxyl group in their molecular structure. These compounds are soluble in highly polar solvents [[21\]](#page-7-0).

3.2. Phytochemical analysis

3.2.1. Anti-nutrients

Phytochemical compounds that have the ability to hamper the nutritional quality of sesame seeds were investigated. Using Equations [\(2\)](#page-2-0)–(5), anti-nutrients such saponins, alkaloids, oxalates, and phytates respectively were quantified. The result obtained is shown in Table 2. The seeds were found to contain high alkaloid content of 317.33 ± 30.29 mg/g (p *<* 0.05), with low levels of oxalates at 1.501 ± 0.1375 mg/g, (p *<* 0.05).

Anti-nutrients are phytochemicals that can decrease the body's ability to absorb essential nutrients [[7](#page-7-0)]. Knowing the nutritional content of our food is essential for a healthy lifestyle. For instance, it has been established that high levels of saponins above 10 % are dangerous for the body as they inhibit growth, reduce the bioavailability of nutrients and prevent biochemical reactions that facilitate the breakdown of proteins in the body [\[16](#page-7-0)]. However, their presence also supports medicinal properties such as anti-inflammatory, antimicrobial, and anti-cancer properties, all related to antioxidant capacity [22–[24\]](#page-7-0). It is therefore important to measure the amount present in our diet. Alkaloids, a well-known therapeutic agent, can also be harmful in high concentrations. Literature reports show that the alkaloid content in sesame seeds is between $(4.80 \text{ mg}/100 \text{ g}-56 \text{ mg/g})$ [[25,](#page-7-0)[26\]](#page-8-0), which means that the alkaloid content of 317.33 mg/g found in research is significantly increased. The amount and type of phytochemicals produced by plants depend on several factors such as temperature, soil conditions, and season(dry or wet season) [\[27](#page-8-0),[28\]](#page-8-0). The high levels of alkaloids content obtained from the study could be attributed to environmental/geographical conditions as well as effect of solvent or method of extraction. Higher concentrations of alkaloids can be toxic [[7\]](#page-7-0). However, reports have shown therapeutic value of alkaloids that enable their use as antitumor, anticancer, anti-inflammatory and antioxidants [\[29](#page-8-0)].

Oxalate in the body combines with calcium and magnesium to form insoluble salts that cannot be absorbed by the body, resulting in kidney stones. Phytates also form insoluble salts with ions of mineral elements such as calcium, magnesium, zinc and iron, reducing their bioavailability in the body and leading to mineral deficiencies [[16,](#page-7-0)[30\]](#page-8-0). The present study showed a low oxalate and phytate content compared to the data available in the literature [[31\]](#page-8-0). The low level of oxalates and phytates in this study means that the sesame seeds used in the study are less likely to reduce bioavailability of nutrient when consumed, compared to the once used in other studies. Again, it has been reported that levels of these anti-nutrient compounds decrease during processing such as fermentation, maceration and heating [[29,32\]](#page-8-0). Data obtained from the study shows that sesame seeds have good nutritional quality.

3.3. Antioxidant activity assays

3.3.1. Total phenolic content and condensed tannin content

The effects of different solvent types on phytochemical components and their associated antioxidant properties were analysed and the results are shown in Table 3. The aqueous extract exhibited the highest TPC (17.12 ± 0.041 mg GAE/g of dried extract, p *<* 0.05)

Fig. 1. DPPH free radical scavenging activity of extracts and ascorbic acid.

Fig. 2. Bivariate Pearson's correlation matrix plot of TPC, CTC, TAC and DPPH.

and CTC (64.27 ± 4.711 mg CE/g of dried extract, p *<* 0.05). Ethanol and hexane had a similar total phenolic content (14.83 ± 0.123 and 14.66 ± 1.474 mg GAE/g of dried extract, respectively, p *<* 0.05Ethyl acetate had the lowest TPC content.

The results ([Table 3\)](#page-4-0) show that the ethanolic extract has the highest total antioxidant capacity (232.6 \pm 6.267 mg AAE/g dry extract. According to literature [[33\]](#page-8-0), alkaloids and other polar and medium polar compounds are extracted using methanol or ethanol. Thus the high antioxidant capacity observed from the ethanol extract could be a result of the presence of extremely high alkaloid content, significantly high phenolic contents and synergistic effect of other compounds that also have antioxidant capacities. A significant antioxidant was observed in the other solvent extract because, sesame is rich in phytosterols and tocopherols [\[25\]](#page-7-0), which are soluble in a polar solvents such as hexane. Scientists attribute the antioxidant effects of these phytosterols to the formation of the allyl radical and its isomerization into other relatively stable free radicals [[34\]](#page-8-0). Additionally, hexane solvents have been reported to extract terpenoid-derived compounds that are essential for improving human health. Terpenoid-derived compounds are also known to provide provitamin A or β-carotene, a compound believed to be found in sesame [[3](#page-7-0)].

Considering the radical scavenging activity, it was observed that the inhibition activity of the extracts increased with increasing concentration. The percentage inhibition was estimated using Equation (6) and the plot shown in Fig. 1.

3.4. Chemometric analysis

To examine the relationships between the measured variables, a comparative analysis (Pearson correlation) was performed. The results of the analysis are shown in Fig. 2 and [Table 4](#page-6-0). A strong negative linear correlation coefficient was observed between TAC and DPPH (− 0.784). TPC was weakly correlated with TAC (− 0.387) and DPPH (− 0.253), which implied that the total phenol content was

Table 4

Bivariate Pearson's correlation coefficients (R) between total phenolic, condensed tannin content, total antioxidant capacity, and DPPH radical scavenging activity of the extracts tested from *S. indicum*.

Fig. 3. The dendrogram obtained by hierarchical cluster analysis using Ward's method and the squared Euclidean distance metric. For data of TPC, CTC, TAC, DPPH, and percentage yield of extraction of the extracts. SA, '*Sesamum indicum* aqueous extract'; SE, *Sesamum indicum* ethanolic extract; SETAC, "*Sesamum indicum* ethyl acetate extract'; SH, "*Sesamum indicum* hexane extract'.

not a major contributing factor to the high total antioxidant capacity and the free radical scavenging property. This could be as a result of other components found in the seeds of the plant which are not phenolic but exhibit antioxidant property. In addition, a cluster analysis was used to provide information about the associations and patterns in the data obtained. The dendrogram obtained from the unsupervised hierarchical cluster analysis Fig. 3 displayed a certain correlation among the various extracts in the study. The analysis of the results showed that the extracts created a non-homogeneous data set. Three different clusters (C1–C3) were generated. SH and SE were found in a group characterized by high antioxidant capacity and strong free radical scavenging capacity. SA belonged to the second group characterized by high TPC content, low antioxidant capacity and low free radical scavenging capacity. In the third group, SETAC was found, which was characterized by low phenol content and low antioxidant activity.

Using the Pearson correlation Fig. 3 and Table 4, the relationship between TPC, CTC and TAC in various plant extracts was determined to determine the contribution of these variables in the extracts to their overall antioxidant activity [[14\]](#page-7-0). Total phenol content has been used as an indicator of the antioxidant properties of plant extracts and has been repeatedly reported in the literature. Parikh and Patel, 2018, reported a strong positive correlation (p *<* 0.01) between TPC and TAC in the determination of total phenolic content and total antioxidant capacity of common Indian legumes and split legumes [[27\]](#page-8-0). Other studies also found a high positive correlation between total antioxidant capacity and phenol content [[28,35\]](#page-8-0). However, Luta and co-workers have reported a negative correlation between total phenol content and DPPH scavenging activity of Hippophae rhamnoides L. Berries [[36\]](#page-8-0). Additionally, Ruslan and colleagues also found a negative correlation between TPC in black sesame seed extract and IC50-ABTS value (r = − 0.828, p *<* 0.01) [\[37](#page-8-0)]. However, the current study showed no significant connection between the radical scavenging activity of TPC and DPPH. This is in agreement with other studies reported in the literature $[28,38,39]$ $[28,38,39]$ $[28,38,39]$ $[28,38,39]$. The high antioxidant activity recorded by sesame seeds may be due to other phytochemicals such as carotenoids [[40\]](#page-8-0), antioxidant polypeptides [\[41](#page-8-0)] and vitamins C and/or E, since sesame seeds contains high levels these lipid soluble compounds.

3.5. Conclusions

The study confirms the presence of different bioactive compounds, such as tannins, phenolics and alkaloids in sesame seed extracts which explains why it has been used by used as an important ingredient in traditional Chinese medicine, nutraceuticals and other pharmaceutical products. According to the study, the bioactive compounds present in the sesame seed and their subsequent antioxidant properties are dependent on the nature of the solvent used for extraction. The high alkaloids in the study paves way for further research to isolate the alkaloids, and determine their cytotoxicity.

Data availability statement

All data are presented in this manuscript, however, data obtained from the study will be available upon request.

CRediT authorship contribution statement

Mercy Badu: Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition, Conceptualization. **Gilsonda Akweley Kordei Attuquaye:** Writing – original draft, Investigation, Formal analysis, Data curation. **Azanlerigo Emmanuel:** Writing – original draft, Investigation, Formal analysis, Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References

- [1] [J. Dai, R.J. Mumper, Plant phenolics: extraction, analysis and their antioxidant and anticancer properties, Molecules 15 \(2010\) 7313](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref1)–7352.
- [2] [M. Olszowy, What is responsible for antioxidant properties of polyphenolic compounds from plants? Vol. 144, Plant Physiol. Biochem. \(2019\) 135](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref2)–143.
- [3] [F. Moghtaderi, N. Ramezani-Jolfaie, H. Raeisi-Dehkordi, A. Salehi-Abargouei, Sesame seed and its fractions for improving oxidative stress in adults: a systematic](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref3) [review and meta-analysis of controlled clinical trials, Food Rev Int \[Internet\] 36 \(8\) \(2020\) 727](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref3)–744. Available from:.
- [4] [M. Yu, I. Gouvinhas, J. Rocha, A.I.R.N.A. Barros, Phytochemical and antioxidant analysis of medicinal and food plants towards bioactive food and](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref4) [pharmaceutical resources, Sci. Rep. 11 \(2021\).](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref4)
- [5] [C.K.B. Ferrari, E.A.F.S. Torres, Biochemical pharmacology of functional foods and prevention of chronic diseases of aging, Biomed. Pharmacother. 57 \(5](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref5)–6) [\(2003\) 251](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref5)–260.
- [6] [K. Rani, Role of antioxidants in prevention of diseases, J Appl Biotechnol Bioeng. 4 \(1\) \(2017\).](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref6)
- [7] [Gemede H. Fekadu, Antinutritional factors in plant foods: potential health benefits and adverse effects, Int. J. Nutr. Food Sci. 3 \(4\) \(2014\) 284.](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref7)
- [8] [M. Badu, M.-M. Pedavoah, N.O. Boadi, I.Y. Dzaye, Proximate composition, in vitro antioxidant and anti-inflammatory properties of Adansonia digitata and](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref8) [belanites aegyptiaca seeds, J Trop Pharm Chem. 5 \(4\) \(2021\) 286](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref8)–298.
- [9] [C. Di Lorenzo, F. Colombo, S. Biella, C. Stockley, P. Restani, Polyphenols and human health: the role of bioavailability, Nutrients 13 \(1\) \(2021\) 1](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref9)–30.
- [10] [M.D. Kontogianni, A. Vijayakumar, C. Rooney, R.L. Noad, K.M. Appleton, D. McCarthy, et al., A high polyphenol diet improves psychological well-being: the](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref10) [polyphenol intervention trial \(pphit\), Nutrients 12 \(8\) \(2020\) 1](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref10)–16.
- [11] E.E. Özdemir, A. Görgüç, E. Gençdağ, F.M. Yılmaz, Physicochemical, functional and emulsifying properties of plant protein powder from industrial sesame [processing waste as affected by spray and freeze drying, Lwt 154 \(2022\).](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref11)
- [12] [S. Abbas, M.K. Sharif, M. Sibt-E-Abbas, T. Fikre Teferra, M.T. Sultan, M.J. Anwar, Nutritional and therapeutic potential of sesame seeds, J. Food Qual. 2022](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref12) [\(2022\).](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref12)
- [13] [T. Cells, Anticancer properties of in investigation of wound healing and anticancer properties of in vitro grown sesame plant extract in L929 , A549 , and MCF-7](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref13) [cell lines and transcriptomic analyses of Cas3 , Cas9, BCL-XL Genes in the Sesame Extract Treat \(2023\)](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref13).
- [14] [A. Wakeel, S.A. Jan, I. Ullah, Z.K. Shinwari, M. Xu, Solvent polarity mediates phytochemical yield and antioxidant capacity of Isatis tinctoria, PeerJ 2019 \(10\)](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref14) [\(2019\) 1](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref14)–19.
- [15] [A. Yadav, R. Kumari, A. Yadav, J.P. Mishra, S. Srivatva, S. Prabha, A. Yadav, R. Kumari, A. Yadav, J.P. Mishra, S. Srivatva, S. Prabha, Antioxidants and its](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref15) [functions in human body-A Review, Res Environ Life Sci. 2016 9 \(11\) \(2016\) 1328](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref15)–1331.
- [16] [J.O. Unuofin, G.A. Otunola, A.J. Afolayan, Nutritional evaluation of Kedrostis africana \(L.\) Cogn: an edible wild plant of South Africa, Asian Pac. J. Trop.](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref16) [Biomed. 7 \(5\) \(2017\) 443](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref16)–449.
- [17] R. Nagy, E. Szőllősi, P. Bíróné Molnár, E. Murányi, R. Czimbalmos, P. Sipos, Condensed tannin content and antioxidant activity of Hungarian sorghum varieties [grown at Research Institute in Karcag, Acta Agrar Debreceniensis \(1\) \(2021\) 155](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref17)–160.
- [18] [Frempong T. Fadjare, N. Owusu Boadi, M. Badu, Optimization of extraction conditions for polyphenols from the stem bark of Funtumia elastica \(Funtum\)](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref18) [utilizing response surface methodology, AAS Open Res 4 \(2021\) 46](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref18).
- [19] [T.N. Minh, T.D. Xuan, H.D. Tran, T.M. Van, Y. Andriana, T.D. Khanh, et al., Isolation and purification of bioactive compounds from the stem bark of Jatropha](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref19) [podagrica, Molecules 24 \(5\) \(2019\) 1](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref19)–15.
- [20] [C. Cravotto, A.S. Fabiano-Tixier, O. Claux, M. Abert-Vian, S. Tabasso, G. Cravotto, et al., Towards substitution of hexane as extraction solvent of food products](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref20) [and ingredients with No regrets, Foods 11 \(21\) \(2022\)](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref20).
- [21] [C. Sun, Z. Wu, Z. Wang, H. Zhang, Effect of ethanol/water solvents on phenolic profiles and antioxidant properties of Beijing propolis extracts, Evid. base Compl.](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref21) [Alternative Med. 2015 \(2015\).](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref21)
- [22] [S.G. Sparg, M.E. Light, J. Van Staden, Biological activities and distribution of plant saponins, J. Ethnopharmacol. 94 \(2](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref22)–3) (2004) 219–243.
- [23] [G. Francis, Z. Kerem, H.P.S. Makkar, K. Becker, The biological action of saponins in animal systems: a review, Br. J. Nutr. 88 \(6\) \(2002\) 587](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref23)–605.
- [24] [M. Marrelli, F. Conforti, F. Araniti, G.A. Statti, Effects of saponins on lipid metabolism: a review of potential health benefits in the treatment of obesity,](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref24) [Molecules 21 \(10\) \(2016\)](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref24).
- [25] [B. Mbaebie, G. Omosun, A. Uti, S. Oyedemi, Chemical composition of Sesamum indicum L. \(Sesame\) grown in Southeastern Nigeria and the physicochemical](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref25) [properties of the seed oil, Seed Sci. Biotechnol. 4 \(1\) \(2010\) 69](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref25)–72.
- [26] [N.C. Samuel, A.C. Genevieve, Proximate analysis and phytochemical properties of sesame \(Sesamum indicum L.\) seeds grown and consumed in abakaliki,](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref26) [ebonyi state, Nigeria, Int J Heal Med 2 \(4\) \(2017 Dec 29\) 1](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref26).
- [27] B. Parikh, V.H. Patel, Total phenolic content and total antioxidant capacity of common Indian pulses and split pulses, J Food Sci Technol [Internet] 55 (4) (2018 Apr 5) 1499–1507. Available from: [http://link.springer.com/10.1007/s13197-018-3066-5.](http://link.springer.com/10.1007/s13197-018-3066-5)
- [28] E. Balogh, A. Hegedus, É. Stefanovits-Bányai, [Application of and correlation among antioxidant and antiradical assays for characterizing antioxidant capacity of](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref28) [berries, Sci. Hortic. \(Amst.\) 125 \(3\) \(2010\) 332](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref28)–336.
- [29] [W.A. Jimoh, O.A. Fagbenro, E.O. Adeparusi, Effect of processing on some minerals, anti-nutrients and nutritional composition of sesame \(Sesamum indicum\)](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref29) [seed meals, Electron. J. Environ. Agric. Food Chem. 10 \(1\) \(2011\) 1858](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref29)–1864.
- [30] [S.M.G. Pires, R.S. Reis, S.M. Cardoso, R. Pezzani, E. Paredes-Osses, A. Seilkhan, et al., Phytates as a natural source for health promotion: a critical evaluation of](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref30) [clinical trials, Front. Chem. 11 \(April\) \(2023\) 1](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref30)–11.
- [31] [Z. Jaradat, A Al Aboudi, M. Shatnawi, Q. Ababneh, J. Microbiol. Biotechnol. Food Sci. 2 \(6\) \(2013\) 2455](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref31)–2461.
- [32] A.O. M, K.-K.D. B, I.E. M, Anti-nutrients, bioaccessibility and mineral balance of cookies produced from processed sesame seed flour blends, Int J Food Sci Nutr Eng [Internet] 2020 (1) (2020) 1–11. Available from:<http://journal.sapub.org/food>.
- [33] [Y Bin Ji, X. Han, S.T. Wang, Q.C. Dai, P. Tian, Research on the extraction Technology of alkaloids in natural medicine, Appl. Mech. Mater. 411](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref33)–414 (2013) [3218](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref33)–3222.
- [34] [N. Pathak, A.K. Rai, R. Kumari, K.V. Bhat, Value addition in sesame: a perspective on bioactive components for enhancing utility and profitability, Phcog. Rev. 8](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref34) [\(16\) \(2014\) 147](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref34)–155.
- [35] [A.I. Osorio-Valencia, J. de Jesús Franco-Mejía, J.A. Hoyos-Arbel](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref35)áez, L. Blandón-Naranjo, O.A. Vega-Castro, J. del Carmen Contreras-Calderón, Evaluation of [antioxidant capacity in different food matrices through differential pulse voltammetry and its correlation with spectrophotometric methods, J Appl Electrochem](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref35) [\[Internet\] 53 \(12\) \(2023\) 2495](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref35)–2505. Available from:
- [36] G. Luță, F. Israel-Roming, D. Bălan, E. Gherghina, ESTIMATINGFREERADICALS SCAVENGINGACTIVITYOFSOMEBERRIESSPECIES XVII [\(2013\) 61](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref36)–64.
- [37] [K. Ruslan, S. Happyniar, I. Fidrianny, Antioxidant potential of two varieties of Sesamum indicum L. collected from Indonesia, J Taibah Univ Med Sci \[Internet\]](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref37) 13 (3) (2018) 211–[218. Available from:](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref37).
- [38] [S. Ercisli, M. Akbulut, O. Ozdemir, M. Sengul, E. Orhan, Phenolic and antioxidant diversity among persimmon \(Diospyrus kaki L.\) genotypes in Turkey, Int. J.](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref38) [Food Sci. Nutr. 59 \(6\) \(2008\) 477](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref38)–482.
- [39] M.P. Kähkönen, [A.I. Hopia, H.J. Vuorela, J.P. Rauha, K. Pihlaja, T.S. Kujala, et al., Antioxidant activity of plant extracts containing phenolic compounds,](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref39) [J. Agric. Food Chem. 47 \(10\) \(1999\) 3954](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref39)–3962.
- [40] [W. Stahl, H. Sies, Antioxidant activity of carotenoids, Mol. Aspect. Med. 24 \(2003\) 345](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref40)–351.
- [41] [N. Ye, P. Hu, S. Xu, M. Chen, S. Wang, J. Hong, et al., Preparation and characterization of antioxidant peptides from carrot seed protein, J. Food Qual. 2018](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref41) [\(2018\).](http://refhub.elsevier.com/S2405-8440(24)11099-7/sref41)